

Nanobarometers: *In-Situ* Diagnostics for High-Pressure Experiments



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The mechanistic understanding of high-pressure phenomena requires the capability to probe the local material response at high spatial resolution using experiments with complex loading history. Such experiments rely heavily on computational simulations for the interpretation of local conditions such as temperature and pressure history. The development of an *in-situ* nanoscaled pressure sensor provides a means to assess the quality of these simulations through the direct measurement of local peak pressure and comparison with simulation.

The diagnostic developed under this project consists of nanoscale sensors that are imbedded within, or in contact with, the medium to be measured. They record the local peak pressure and may be read-out following the experiment using a variety of micro-spectroscopy techniques. The small size of the nanosensors, combined with low volume fractions, limits the influence of the sensors on the high-pressure phenomena being studied while allowing for high spatial

resolution of the peak local pressure. Preliminary work indicates that the fabrication, deployment, and read-out of the nanoscale pressure sensors are possible. We are executing a comprehensive plan to explore the scale dependence, concentration limits, and pressure sensitivity of nanoscale pressure sensors. The final product shall be an *in-situ* nanoscale pressure sensing capability that has been calibrated over a wide range of pressures (from 30 to 300 kbar) and a range of deformation conditions from quasi-static to weak shocks. The development of an *in-situ*, nanoscale pressure sensor will provide both a valuable tool for many existing high-pressure applications and an enabling technology for new uses and novel experiments; thus complementing many existing Laboratory programs in nanoscale modeling, material failure and fracture, and laser-driven experiments. A natural extension would be to design new materials to extend the useful pressure range of the proposed sensors to both lower and higher pressures.

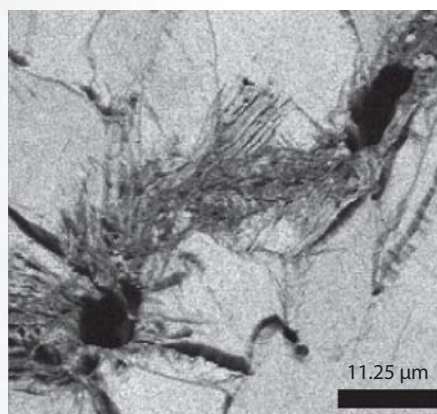


Figure 1. Micrograph of incipiently spalled and recompressed copper sample.

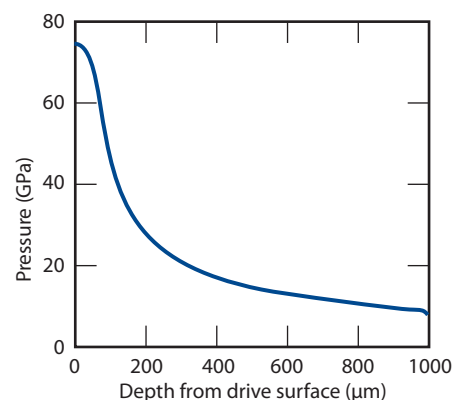


Figure 2. Computed peak pressure profile due to a laser-driven shock.

Project Goals

The project goal is to develop an *in-situ* diagnostic for high-pressure experiments capable of providing local peak pressure information at high resolution ($<1\ \mu\text{m}$) and over a broad range of pressure (30 to 300 kbar). Key issues to be addressed shall include calibration and sensitivity analysis of the nanosensors to quasi-static conditions. Major goals of the proposed research are to quantify the extent of pressure induced changes in the sensor material, determine their dependence on sensor size, and establish the sensitivity of pressure induced structural changes to static loading.

Relevance to LLNL Mission

The study of high-pressure phenomena is at the core of many DNT and NIF related programs, with many important applications in the range of a few hundred kilobars, such as fragmentation and spall. Such experiments rely heavily on computational simulations for the interpretation of local conditions such as temperature and pressure history. The development of an *in-situ* nanoscaled pressure sensor provides a means to assess the quality of these simulations through the direct measurement of local peak pressure and comparison with simulation. Such a capability is especially useful in laser-driven experiments with complex wave profiles and non-steady

loading. The proposed nanosensors complement many existing Laboratory programs in multi-scale modeling, material failure and fracture, and laser-driven experiments. Potential application to three classes of experiments is envisioned: Quasi-Static Experiments in Bulk Materials, Unsteady Shocks in Bulk Materials, and High Explosives. From gas-gun and laser-driven experiments to Site 300 and NTS U1a test shots, there is a need for an accurate, local measure of material peak pressure.

FY2006 Accomplishments and Results

Figures 1-4 illustrate our results. A key question regarding the existence and nature of the densification mechanism in silica nanoparticles has been explored. The issue was whether or not the densification phenomena observed in bulk silica occurred in nanoparticles. Since the success of the entire project is predicated upon this, it was crucial to experimentally verify this assertion. The results of a series of Raman spectroscopy and diamond anvil experiments on silica nanoparticles are quite intriguing. The permanent shift in the Raman spectra is clearly visible, consistent with the published results in bulk silica glass. To the best of our knowledge, this is the first such measurement in nanoparticles as a function of particle size. Not unexpected is the dependence of the

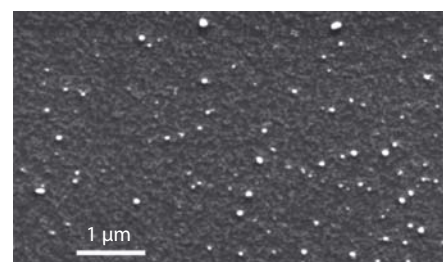


Figure 4. Micrograph of sub-micron silica sensors embedded in a copper matrix.

Raman shift upon the particle size, a key research question to be addressed by this project. Results obtained this last year show, as suspected, a clear change in the size dependence for the smallest particles ($< 80\ \text{nm}$ in Fig. 3). Note that each experimental point represents an entire sequence of spectra taken upon loading and unloading of each sample. As a consequence of the success of this year's experiments a record of invention has been filed and a preliminary patent is being pursued.

Related References

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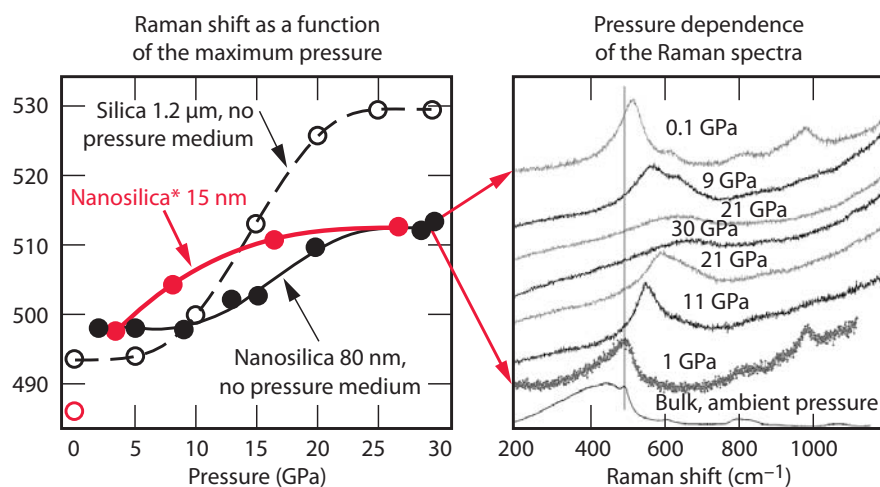


Figure 3. Permanent shift in Raman spectra as function of peak pressure and particle size (15, 80, and 1200 nm). 15 nm particles show distinctly different pressure dependence.